

PCA with Gaussian perturbations

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Abstract

Most of machine learning deals with vector parameters. Ideally we would like to take higher order information into account and make use of matrix or even tensor parameters. However the resulting algorithms are usually inefficient. Here we address on-line learning with matrix parameters. It is often easy to obtain online algorithm with good generalization performance if you eigendecompose the current parameter matrix in each trial (at a cost of $O(n^3)$ per trial). Ideally we want to avoid the decompositions and spend $O(n^2)$ per trial, i.e. linear time in the size of the matrix data. There is a core trade-off between the running time and the generalization performance, here measured by the regret of the on-line algorithm (total gain of the best off-line predictor minus the total gain of the on-line algorithm).

We focus on the key matrix problem of rank k Principal Component Analysis in \mathbf{R}^n where $k \ll n$. There are $O(n^3)$ algorithms that achieve the optimum regret but require eigendecompositions. We develop a simple algorithm that needs $O(kn^2)$ per trial whose regret is off by a small factor of $O(n^{1/4})$. The algorithm is based on the Follow the Perturbed Leader paradigm. It replaces full eigendecompositions at each trial by the problem finding k principal components of the current covariance matrix that is perturbed by Gaussian noise.

1. Introduction

In Principal Component Analysis (PCA), the data points $\mathbf{x}_t \in \mathbb{R}^n$ are projected onto a k -dimensional subspace (represented by a rank k projection matrix \mathbf{P}). The goal is to maximize the total squared norm of the projected data points, $\sum_t \|\mathbf{P}\mathbf{x}_t\|^2$. This is equivalent to finding the *principal* eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ i.e. those belonging to the k largest eigenvalues of the data “covariance matrix” $\sum_t \mathbf{x}_t \mathbf{x}_t^\top$, and setting the projection matrix to $\mathbf{P} = \sum_{i=1}^k \mathbf{u}_i \mathbf{u}_i^\top$. In this paper we choose the online version of PCA (Warmuth and Kuzmin, 2008) as our paradigmatic matrix parameter problem and we explore the core trade-off between generalization performance and time efficiency per trial for this problem. In each trial $t = 1, \dots, T$, the online PCA algorithm chooses a projection matrix \mathbf{P}_t of rank k based on the previously observed points $\mathbf{x}_1, \dots, \mathbf{x}_{t-1}$. Then a next point \mathbf{x}_t is revealed and the algorithm receives gain $\|\mathbf{P}_t \mathbf{x}_t\|^2$. The goal here is to obtain an online algorithm whose cumulative gain over trials $t = 1, \dots, T$ is close to the cumulative gain of the best rank k projection matrix chosen in hindsight after seeing all T instances. The maximum difference between the cumulative gain of the best off-line comparator and the cumulative gain of the algorithm and is called the (worst-case) *regret*.

If you use the principal eigenvectors \mathbf{u}_i ($1 \leq i \leq k$) as the parameters, then the gain is formidably non-convex. However the key insight of (Warmuth and Kuzmin, 2006, 2008) is the observation that the seemingly quadratic gain $\|\mathbf{P}\mathbf{x}_t\|^2$ is a *linear function* of the projection matrix \mathbf{P} when the data is expressed in terms of the *matrix instance* $\mathbf{x}_t\mathbf{x}_t^\top$ rather than vector instance \mathbf{x}_t :

$$\|\mathbf{P}\mathbf{x}_t\|^2 = \mathbf{x}_t \mathbf{P}^2 \mathbf{x}_t \stackrel{\mathbf{P}^2 = \mathbf{P}}{=} \mathbf{x}_t \mathbf{P} \mathbf{x}_t = \text{tr}(\mathbf{P} \mathbf{x}_t \mathbf{x}_t^\top).$$

Good algorithms hedge their bets by predicting with a random projection matrix. In that case $\mathbb{E}[\|\mathbf{P}\mathbf{x}_t\|^2]$ becomes $\text{tr}(\mathbb{E}[\mathbf{P}] \mathbf{x}_t \mathbf{x}_t^\top)$. Thus it is natural to use mixtures $\mathbb{E}[\mathbf{P}]$ of rank k projection matrices as the parameter matrix of the algorithm. Such mixture are positive definite matrices of trace k with eigenvalues capped at 1. The gist is that the gain is now linear in this alternate parameter matrix and the non-convexity has been circumvented. This observation is the starting point for lifting known online learning algorithms for linear gain/loss on vector instances to the matrix domain, which resulted in the Matrix Exponentiated Gradient (MEG) algorithm (Tsuda et al., 2005; Arora and Kale, 2007; Warmuth and Kuzmin, 2008), as well as the (matrix) Gradient Descent (GD) algorithm (Arora et al., 2013, 2012; Jiazhong et al., 2013). Both algorithms are motivated by trading off a Bregman divergence against the gain, followed by a Bregman projection onto the convex hull of rank k projection matrices which is our parameter space. The worst-case regret of these algorithms for online PCA is optimal (within constant factors). Furthermore MEG remains optimal for a generalization of the PCA problem to the *dense instance* case in which the “sparse” rank one outer products $\mathbf{x}_t \mathbf{x}_t^\top$ of vanilla PCA are generalized to positive definite matrices \mathbf{X}_t with bounded eigenvalues. (Jiazhong et al., 2013).

Unfortunately, both algorithms require full eigendecomposition of the parameter matrix at a cost of $O(n^3)$ per trial.¹ It was posed as an open problem (Hazan et al., 2010) whether there exists an algorithm with good regret guarantees requiring time comparable with that of finding the top k eigenvectors. The latter operation can be done efficiently by means of e.g. power iteration based methods (Arnoldi, 1951; Cullum and Willoughby, 1985): It essentially requires time $O(kn^2)$, which is much less than the cost of a full eigendecomposition in the natural case when $k \ll n$. This operation is also used by the simple *Follow the Leader* algorithm which predicts with the k principal components of the current covariance matrix. This algorithm performs well when the data is i.i.d. but can be forced to have large regret on worst-case data.

In this paper, we provide an algorithm based on the *Follow the Perturbed Leader* (FPL) approach, which perturbs the cumulative data matrix by adding a random symmetric noise matrix, and then predicts with the k principal components of the current perturbed covariance matrix. The key question is what perturbation to use and whether that exists a perturbation for which FPL achieves close to optimal regret. In the vanilla vector parameter based FPL algorithm (Kalai and Vempala, 2005), exponentially distributed perturbation lead to optimal algorithms when the perturbations is properly scaled. We could apply the same perturbations to the eigenvalues of the current parameter matrix and achieve optimal regret. However this approach requires us to eigendecompose the current parameter matrix

1. For the rank one instances $\mathbf{x}_t \mathbf{x}_t^\top$ of PCA the update of the eigenvalues takes $O(n^2)$ Bunch et al. (1978/79) per trial. However the update of the eigensystem remains $O(n^3)$.

and this defeats the purpose. We need to find a perturbation that requires $O(n^2)$ time to compute instead of $O(n^3)$. We use a random symmetric Gaussian matrix (a so called *Gaussian orthogonal ensemble*), which consists of entries generated i.i.d. from a Gaussian distribution. Our approach is more similar to the recent algorithm based on *Random Walk Perturbation* Devroye et al. (2013) and can be considered as a matrix generalization thereof, drawing connections to Random Matrix Theory Tao (2012). Calculation of our random noise matrix requires $O(n^2)$ and hence the total computational time is dominated by finding the k principal components of the perturbed matrix. At the same time, our algorithm achieves $O(n^{1/4}\sqrt{kT})$ worst-case regret for online PCA (sparse instances) and $O(k\sqrt{nT})$ worst-case regret for dense instance case. Comparing to the minimax regrets $\Theta(\sqrt{kT})$ and $\Theta(k\sqrt{T\log n})$ in the sparse and dense cases, respectively, we are only a factor of $O(n^{1/4})$ and $O(n^{1/2})$ off from the optimum, respectively.

Our approach can be considered a generalization of the *Random Walk Perturbation* (RWP) algorithm Devroye et al. (2013) to the matrix domain. In RWP, an independent Bernoulli coin flip is added to each component of the loss/gain vector, the process which can be closely approximated (through Central Limit Theorem) by Gaussian perturbations with variance growing linearly in t . This is also the case of our algorithm, where we use a symmetric matrix with i.i.d. Gaussian-distributed entries with variance also growing linearly in t . Our analysis, however, resorts to properties of random matrices, e.g. expected maximum eigenvalue, which leads to worse regret bounds than in the vector case. Interestingly, comparing to Devroye et al. (2013) we get rid of additional $O(\log T)$ factor in the regret.

Related work. Online PCA, in the framework considered here, was introduced in Tsuda et al. (2005) and independently in Arora and Kale (2007), along with Matrix Exponentiated Gradient algorithm. The problem of finding efficient algorithms which avoid full eigendecomposition was posed as an open problem by Hazan et al. (2010). An efficient algorithm for PCA based on Online Gradient Descent was proposed in Arora et al. (2013, 2012), but the main version of the algorithm (*Matrix Stochastic Gradient, MSG*) still requires $O(n^3)$ in the worst case, while a faster version (*Capped MSG*) operates on low-rank deterministic parameter matrix, which can be shown to have regret linear in T in the adversarial setting. The most closely related to our work is Garber et al. (2015), in which several algorithms are proposed for learning the top eigenvector (i.e., the simplest case $k = 1$ of online PCA): based on online Franke-Wolfe method Hazan and Kale (2012), and based on FPL approach with entry-wise uniform perturbation, exponentially-distributed perturbation, and a perturbation based on a sparse rank-one random matrix $\mathbf{v}\mathbf{v}^\top$ composed of a random Gaussian vector \mathbf{v} . Except for the last algorithm, all the other approaches have regret guarantees which are inferior comparing to our method, either in terms of dependence on T or dependence on n , or both. The method based on rank-one perturbation achieves regret bound $O(\sqrt{nT})$ which is the same as ours in the dense instance case. It is not clear whether this method would benefit anyhow from sparsity of instance matrices (as in the standard online PCA), and whether it would easily generalize to $k > 1$ case.

There are other formulations of online PCA problem. For instance, Boutsidis et al. (2015) aims at finding low dimensional data representation in a single pass, with the goal of good reconstruction guarantees using only a small number of dimensions. On the other

hand, Balsubramani et al. (2013); Shamir (2015) consider online PCA in the stochastic optimization setting. However, the algorithm considered therein are not directly applicable in the adversarial setting studied in this work.

New conjecture. Our algorithm is efficient, but its suboptimal regret is due to the fact that the noise matrix does not adapt to the eigensystem of cumulative covariance matrix. What $O(n^2)$ perturbation can we use that does adapt to the eigensystem of the current covariance matrix? A clear candidate is to use *Dropout Perturbation*. In the vector case this perturbation independently at random zeros out each component of the gain/loss vector in each trial (van Erven et al., 2014) and achieves optimal regret without having to tune the magnitude of the perturbations. In the matrix case it would be natural to independently zero out components of the instance matrix when expressed in the eigensystem of the current loss matrix. However these approaches again require eigendecompositions.

A new variant is to skip at trial t the entire instance matrix with probability half, i.e. at trial t predict with the k principal components of the following perturbed current covariance matrix

$$\sum_{q=1}^{t-1} \alpha_t \mathbf{X}_t,$$

where the α_t are Bernoulli coin flips with probability half. We call this the *Follow the Skipping Leader* algorithm because it skips entire instances \mathbf{X}_t with probability half. It is easy to maintain this perturbed covariance matrix in $O(n^2)$ time per trial. However, unfortunately already in the vector parameter case this algorithm can be forced to have a gravely suboptimal linear regret in n (Neu and Lugosi, 2014). The counter example requires dense loss vectors. When lifting this counter example to the matrix setting then the regret can still be forced to be linear with sparse instance $\mathbf{x}_t \mathbf{x}_t^\top$. However we conjecture that the time efficient Follow the Skipping Leader algorithm achieves the optimal regret for standard PCA with sparse instance. This is because in PCA regret is naturally measured w.r.t. the maximum gain of the best rank k subspace and not the loss. Note that that this type of problem is decidedly not symmetric w.r.t. gain and loss (See Jiazhong et al. (2013) for an extended discussion).

Finally we also conjecture the regret bounds achieved by the algorithm of this paper (Gaussian perturbations) is the best you can achieve with rotation invariant noise and knowing this fact would be interesting in its own right.

2. Problem setting

In the online PCA, in each trial $t = 1, \dots, T$, the algorithm probabilistically chooses a projection matrix $\mathbf{P}_t \in \mathbb{R}^{n \times n}$ of rank k . Then a point $\mathbf{x}_t \in \mathbb{R}^n$ is revealed and the algorithm receives *gain* $\|\mathbf{P}_t \mathbf{x}_t\|^2 = \text{tr}(\mathbf{P}_t \mathbf{x}_t \mathbf{x}_t^\top)$. Note again that the gain is linear in \mathbf{P}_t and in *instance matrix* $\mathbf{x}_t \mathbf{x}_t^\top$. This observation calls for generalization of the online PCA in which the instance matrix is any positive definite matrix \mathbf{X}_t (with bounded eigenvalues) and the gain becomes $\text{tr}(\mathbf{P}_t \mathbf{X}_t)$. We call this the *dense instance* case as opposed to standard online PCA, which we call *sparse instance* case.

In the above protocol, the algorithm is allowed to choose its k dimensional subspace \mathbf{P}_t probabilistically. Therefore we use expected gain $\mathbb{E}[\text{tr}(\mathbf{P}_t \mathbf{X}_t)]$ as the evaluation of the algo-

rithm's performance, where the expectation is with respect to the internal randomization of the algorithm. The *regret* of the algorithm is then the difference between the cumulative gain of the best off-line rank k projector and the the cumulative gain of the algorithm (due to linearity of gain, no randomization is necessary when considering the best off-line comparator):

$$\mathcal{R} = \max_{P \in \mathcal{P}} \left\{ \sum_{t=1}^T \text{tr}(\mathbf{P} \mathbf{X}_t) \right\} - \sum_{t=1}^T \mathbb{E}[\text{tr}(\mathbf{P}_t \mathbf{X}_t)] = \lambda_{1:k}(\mathbf{X}_{\leq T}) - \sum_{t=1}^T \mathbb{E}[\text{tr}(\mathbf{P}_t \mathbf{X}_t)], \quad (1)$$

where \mathcal{P} denotes the set of all rank k projectors, $\mathbf{X}_{\leq t} = \sum_{q=1}^t \mathbf{X}_q$ is the cumulative data matrix, and $\lambda_{1:k}(\mathbf{X}) = \sum_{i=1}^k \lambda_i(\mathbf{X})$ denotes the sum of top k eigenvalues of \mathbf{X} . The goal of the algorithm is to have small regret for any sequence of instance matrices. Since the regret naturally scales with the eigenvalues of \mathbf{X}_t , we assume for the sake of simplicity that all eigenvalues of \mathbf{X}_t are bounded by 1 (i.e. for each $t = 1, \dots, T$, the spectral norm of \mathbf{X}_t , $\|\mathbf{X}_t\|_\infty \leq 1$).

We note that due to linearity of the gain, $\mathbb{E}[\text{tr}(\mathbf{P}_t \mathbf{X}_t)] = \text{tr}(\mathbb{E}[\mathbf{P}_t] \mathbf{X}_t)$, so that the algorithm's gain is fully determined by $\mathbb{E}[\mathbf{P}_t]$, a convex combinations of rank k projection matrices. Hence, the parameter set of the algorithm can be equivalently taken as $\mathcal{W} = \text{conv}(\mathcal{P})$, a convex hull of \mathcal{P} , which is a set of positive definite matrices with trace k and all eigenvalues not larger than 1 Warmuth and Kuzmin (2008). This is the key idea behind MEG and GD algorithms, which maintain the uncertainty about projection matrix by means of a parameter $\mathbf{W}_t \in \mathcal{W}$, update their parameter by minimizing a trade-off between a divergence of the new and old parameter and the gain/loss of the new parameter on the current instance, while constraining the new parameter to lie in the parameter set \mathcal{W} . While predicting, the algorithm chooses its projection matrix \mathbf{P}_t by sampling from this mixture \mathbf{W}_t Warmuth and Kuzmin (2008).

3. The algorithm

Our algorithm belongs to a class of *Follow the Perturbed Leader* (FPL) algorithms, which are defined by the choice:

$$\mathbf{P}_t = \underset{\mathbf{P} \in \mathcal{P}}{\text{argmax}} \left\{ \text{tr}(\mathbf{P}(\mathbf{X}_{\leq t} + \mathbf{N}_t)) \right\},$$

where $\mathbf{X}_{\leq t} = \sum_{q \leq t} \mathbf{X}_q$ is the cumulative data matrix observed so far, while \mathbf{N}_t is the symmetric noise matrix generated randomly by the algorithm² and w.l.o.g. we assume $\mathbb{E}[\mathbf{N}_t] = \mathbf{0}$. Perturbing the cumulative data matrix is necessary as one can easily show that any deterministic strategy (including Follow the Leader obtained by taking $\mathbf{N}_t = \mathbf{0}$) can be forced to have regret linear in T .

Define a “fake” prediction strategy:

$$\tilde{\mathbf{P}}_t = \underset{\mathbf{P} \in \mathcal{P}}{\text{argmax}} \left\{ \text{tr}(\mathbf{P}(\mathbf{X}_{\leq t} + \mathbf{N}_t)) \right\},$$

2. Note that if the algorithm plays against *oblivious* adversary, it is allowed to generate the noise matrix once in the first trial and then reuse it throughout the game.

which acts as FPL, but adds the current instance \mathbf{X}_t to the cumulative data matrix, and hence does not correspond to any valid online algorithm. What follows is a standard lemma for bounding the FPL regret, adapted to the matrix case:

Lemma 1 *We have:*

$$\mathcal{R} \leq \sum_t \mathbb{E} \left[\text{tr}((\tilde{\mathbf{P}}_t - \mathbf{P}_t) \mathbf{X}_t) \right] + \sum_t \mathbb{E} [\lambda_{1:k}(\mathbf{N}_t - \mathbf{N}_{t-1})],$$

A vector version of Lemma 1 can be found in standard textbooks on online learning (see, e.g., Cesa-Bianchi and Lugosi (2006)). Since adaptation to the matrix case is rather straightforward, we defer the proof to the Appendix.

We now specify the noise matrix our algorithm employs. Let \mathbf{G} be an $n \times n$ matrix such that each entry is generated i.i.d. from a Gaussian distribution, i.e. $\mathbf{G}_{ij} \sim \mathcal{N}(0, \sigma^2)$. We define the noise matrix of our algorithm as:

$$\mathbf{N}_t = \sqrt{t} \mathbf{N}, \quad \text{where } \mathbf{N} = \frac{1}{2} (\mathbf{G} + \mathbf{G}^\top).$$

Note that \mathbf{N} is a symmetrized version of \mathbf{G} , and \mathbf{N}_t multiplies \mathbf{N} by \sqrt{t} so that the variance of each entry in \mathbf{N}_t grows linearly in t . Interestingly, distribution of \mathbf{N} is known as *Gaussian orthogonal ensemble* in the Random Matrix Theory Tao (2012). The algorithm uses the variable noise rate and hence does not require any tuning for the time horizon T . We still have a single parameter σ^2 , but that parameter is only chosen based on the sparseness of the instance matrix.

Note that according to rules for summing Gaussian variables, we can also express \mathbf{N}_t as a sum of t independent copies of \mathbf{N} , $\mathbf{N}_t = \sum_{q=1}^t \mathbf{N}^{(q)}$. We thus get an equivalent picture of our algorithm in which in each trial, an independent noise variable $\mathbf{N}^{(t)}$ generated from a fixed distribution is added to the current data instance \mathbf{X}_t , and then the action of the algorithm is based on the sum of perturbed data instances. This picture makes our approach similar to RWP algorithm and let us relate our algorithm to dropout perturbation in the next section.

We now show the main result of this paper, the regret bound of the algorithm based on Gaussian perturbation.

Theorem 2 *Given the choice of the noise matrix \mathbf{N}_t described above,*

- *For dense instance, setting $\sigma^2 = 1$ gives:*

$$\mathcal{R} \leq 2k\sqrt{nT}.$$

- *For sparse instance, setting $\sigma^2 = \frac{1}{k\sqrt{n}}$ gives:*

$$\mathcal{R} \leq 2n^{1/4}\sqrt{kT}.$$

Proof We apply Lemma 1 and bound both sums on the right hand side separately. We start with the second sum. We have:

$$\sum_t \mathbb{E} [\lambda_{1:k}(\mathbf{N}_t - \mathbf{N}_{t-1})] = \sum_t (\sqrt{t} - \sqrt{t-1}) \mathbb{E} [\lambda_{1:k}(\mathbf{N})] = \sqrt{T} \mathbb{E} [\lambda_{1:k}(\mathbf{N})]$$

It follows from Random Matrix Theory (see, e.g., Davidson and Szarek (2001)) that the largest eigenvalue of a matrix generated from a Gaussian orthogonal ensemble is of order $O(\sqrt{n})$, specifically:

$$\mathbb{E} [\lambda_{\max}(\mathbf{N})] \leq \sqrt{n\sigma^2}.$$

Therefore,

$$\mathbb{E} [\lambda_{1:k}(\mathbf{N})] \leq k\mathbb{E} [\lambda_{\max}(\mathbf{N})] \leq k\sqrt{n\sigma^2},$$

so that the second sum is bounded by $k\sqrt{nT\sigma^2}$.

Let us now bound the first sum. First, note that $\mathbf{N}_{ij} \sim \mathcal{N}(0, \sigma^2/2)$ for $i \neq j$ and $\mathbf{N}_{ii} \sim \mathcal{N}(0, \sigma^2)$. This means that the joint density $p(\mathbf{N}) = p(\mathbf{N}_{11}, \dots, \mathbf{N}_{nn})$ is proportional to:

$$p(\mathbf{N}) \propto \exp \left\{ -\frac{1}{2\sigma^2} \left(\sum_{i>j} 2\mathbf{N}_{ij}^2 + \sum_i \mathbf{N}_{ii}^2 \right) \right\} = \exp \left\{ -\frac{1}{2\sigma^2} \text{tr}(\mathbf{N}^2) \right\}.$$

Similarly, the joint density of \mathbf{N}_t is proportional to:

$$p_t(\mathbf{N}_t) \propto \exp \left\{ -\frac{1}{2t\sigma^2} \text{tr}(\mathbf{N}_t^2) \right\}.$$

For any symmetric matrix \mathbf{A} , define:

$$\mathbf{P}(\mathbf{A}) = \underset{\mathbf{P} \in \mathcal{P}}{\text{argmax}} \{ \text{tr}(\mathbf{PA}) \},$$

so that $\mathbf{P}_t = \mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t)$ and $\tilde{\mathbf{P}}_t = \mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t + \mathbf{X}_t)$. Furthermore, define a function:

$$f_t(s) = \mathbb{E} [\text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t + s\mathbf{X}_t) \mathbf{X}_t)].$$

Note that $f_t(0) = \mathbb{E} [\text{tr}(\mathbf{P}_t \mathbf{X}_t)]$ and $f_t(1) = \mathbb{E} [\text{tr}(\tilde{\mathbf{P}}_t \mathbf{X}_t)]$. In this notation,

$$\sum_t \mathbb{E} [\text{tr}((\tilde{\mathbf{P}}_t - \mathbf{P}_t) \mathbf{X}_t)] = \sum_t (f_t(1) - f_t(0)),$$

so it remains to bound $f_t(1) - f_t(0)$ for all t . We have:

$$\begin{aligned} f_t(s) &= \int \text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t + s\mathbf{X}_t) \mathbf{X}_t) p_t(\mathbf{N}_t) d\mathbf{N}_t \\ &= \int \text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t) \mathbf{X}_t) p_t(\mathbf{N}_t - s\mathbf{X}_t) d\mathbf{N}_t, \end{aligned}$$

which follows from changing the integration variable from \mathbf{N}_t to $\mathbf{N}_t - s\mathbf{X}_t$. Since by Hölder's inequality:

$$\text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t) \mathbf{X}_t) \leq \text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t)) \cdot \|\mathbf{X}_t\|_\infty = k\|\mathbf{X}_t\|_\infty \leq k, \quad (2)$$

and since p_t is the density of Gaussian distribution, it can easily be shown by using standard argument based on Dominated Convergence Theorem that one can replace the order of

differentiation w.r.t. s and integration w.r.t. \mathbf{N}_t . This means that $f_t(s)$ is differentiable and:

$$\begin{aligned}
 f'_t(s) &= \int \text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t) \mathbf{X}_t) \frac{dp_t(\mathbf{N}_t - s\mathbf{X}_t)}{ds} d\mathbf{N}_t \\
 &= \frac{1}{t\sigma^2} \int \text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t) \mathbf{X}_t) \text{tr}((\mathbf{N}_t - s\mathbf{X}_t) \mathbf{X}_t) p_t(\mathbf{N}_t - s\mathbf{X}_t) d\mathbf{N}_t \\
 &= \frac{1}{t\sigma^2} \int \text{tr}(\mathbf{P}(\mathbf{X}_{} + \mathbf{N}_t + s\mathbf{X}_t) \mathbf{X}_t) \text{tr}(\mathbf{N}_t \mathbf{X}_t) p_t(\mathbf{N}_t) d\mathbf{N}_t \\
 &\leq \frac{r}{t\sigma^2} \int (\text{tr}(\mathbf{N}_t \mathbf{X}_t))_+ p_t(\mathbf{N}_t) d\mathbf{N}_t,
 \end{aligned}$$

where $(c)_+ = \max\{c, 0\}$, and $r = k$ in the dense instance case, while $r = 1$ in the sparse instance case. The last inequality follows from the same argument as in (2) when the instances are dense, and from the opposite application of Hölder's inequality when the instances are sparse, i.e. for sparse instance $\mathbf{X}_t = \mathbf{x}_t \mathbf{x}_t^\top$ with $\|\mathbf{x}_t\| = 1$, and any \mathbf{P} :

$$\text{tr}(\mathbf{P} \mathbf{x}_t \mathbf{x}_t^\top) \leq \text{tr}(\mathbf{x}_t \mathbf{x}_t^\top) \cdot \|\mathbf{P}\|_\infty = \|\mathbf{x}_t\|^2 \cdot 1 = 1.$$

Denote:

$$z = \text{tr}(\mathbf{N}_t \mathbf{X}_t) = 2 \sum_{i>j} (\mathbf{N}_t)_{ij} (\mathbf{X}_t)_{ij} + \sum_i (\mathbf{N}_t)_{ii} (\mathbf{X}_t)_{ii}.$$

Using summation rules for Gaussian variables:

$$z \sim \mathcal{N} \left(0, 2t\sigma^2 \sum_{i>j} (\mathbf{X}_t)_{ij}^2 + t\sigma^2 \sum_i (\mathbf{X}_t)_{ii}^2 \right) = \mathcal{N} \left(0, t\sigma^2 \text{tr}(\mathbf{X}^2) \right),$$

so that:

$$\begin{aligned}
 f'_t(s) &\leq \frac{r}{t\sigma^2} \int (\text{tr}(\mathbf{N}_t \mathbf{X}_t))_+ p_t(\mathbf{N}_t) d\mathbf{N}_t \\
 &= \frac{r}{t\sigma^2} \mathbb{E}_{z \sim \mathcal{N}(0, t\sigma^2 \text{tr}(\mathbf{X}^2))} [(z)_+] \\
 &= \frac{r}{\sqrt{t\sigma^2}} \sqrt{\text{tr}(\mathbf{X}^2)} \mathbb{E}_{z \sim \mathcal{N}(0, 1)} [(z)_+] \\
 &= \frac{r}{\sqrt{2\pi t\sigma^2}} \sqrt{\text{tr}(\mathbf{X}^2)}.
 \end{aligned}$$

By the mean value theorem,

$$f_t(1) - f_t(0) = f'_t(s), \quad \text{for some } s \in [0, 1],$$

which implies:

$$\mathbb{E} \left[\text{tr}((\tilde{\mathbf{P}}_t - \mathbf{P}_t) \mathbf{X}_t) \right] \leq \frac{r}{\sqrt{2\pi t\sigma^2}} \sqrt{\text{tr}(\mathbf{X}_t^2)}.$$

Summing over trials and using $\sum_{t=1}^T 1/\sqrt{t} \leq 2\sqrt{T}$, we bound the first sum in Lemma 1 by $r\sqrt{\frac{2T \max_t \text{tr}(\mathbf{X}_t^2)}{\pi\sigma^2}}$. Using the bound on the second sum, we get that:

$$\mathcal{R} \leq r\sqrt{\frac{2T \max_t \text{tr}(\mathbf{X}_t^2)}{\pi\sigma^2}} + k\sqrt{nT\sigma^2}.$$

The proof is finished by noticing that $\text{tr}(\mathbf{X}^2) \leq n$ and $r = k$ for dense instances, while $\text{tr}(\mathbf{X}^2) = 1$ and $k = 1$ for sparse instances. \blacksquare

Comparing the regret with values of the minimax regret $\Theta(\sqrt{kT})$ in the standard online PCA setting (sparse instance case), and $\Theta(k\sqrt{T \log n})$ in the dense instance case Jiazhong et al. (2013), we see that the algorithm presented here is suboptimal by a factor of $O(n^{1/4})$ in the online PCA setting, and by a factor of $O(\sqrt{n}/\log n)$ in the dense instances setting.

4. Conclusions

In this paper, we studied the online PCA problem and its generalization to the case of dense instance matrices. While there are algorithms which essentially achieve the minimax regret, such as Matrix Exponentiated Gradient or (Matrix) Gradient Descent, all these methods take $O(n^3)$ per trial, because they require full eigendecomposition of the data matrix. We proposed an algorithm based on Follow the Perturbed Leader approach, which uses as a perturbation a random symmetric Gaussian matrix. The algorithm avoids full eigendecomposition and only requires calculating the top k eigenvectors. Hence, prediction takes $O(kn^2)$, while the algorithm achieves the worst-case regret which is only $O(n^{1/4})$ close to the minimax regret for standard online PCA setting, and $O(\sqrt{n})$ close to minimax regret for generalization of online PCA to a dense instance matrices. Finally, we raised an open question, whether a more adaptive version of our algorithm, based on dropout perturbation, would achieve the minimax regret.

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Appendix A. Proof of Lemma 1

We have:

$$\begin{aligned} \lambda_{1:k}(\mathbf{X}_{\leq t} + \mathbf{N}_t) &= \max_{\mathbf{P} \in \mathcal{P}} \{ \text{tr}(\mathbf{P}(\mathbf{X}_{\leq t} + \mathbf{N}_t)) \} \\ &= \text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_{\leq t} + \mathbf{N}_t)) \\ &= \text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_t + \mathbf{N}_t - \mathbf{N}_{t-1})) + \text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_{<t} + \mathbf{N}_{t-1})) \\ &\leq \text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_t + \mathbf{N}_t - \mathbf{N}_{t-1})) + \lambda_{1:k}(\mathbf{X}_{<t} + \mathbf{N}_{t-1}), \end{aligned}$$

so that:

$$\lambda_{1:k}(\mathbf{X}_{\leq t} + \mathbf{N}_t) - \lambda_{1:k}(\mathbf{X}_{<t} + \mathbf{N}_{t-1}) \leq \text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_t + \mathbf{N}_t - \mathbf{N}_{t-1})).$$

Summing over trials $t = 1, \dots, T$, the terms on the left-hand side telescope and, defining $\mathbf{N}_0 = \mathbf{0}$, we get:

$$\lambda_{1:k}(\mathbf{X}_{\leq T} + \mathbf{N}_T) \leq \sum_{t=1}^T \text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_t + \mathbf{N}_t - \mathbf{N}_{t-1})).$$

Since $\lambda_{1:k}(\cdot)$ is convex as a maximum over linear functions, Jensen's inequality implies $\lambda_{1:k}(\mathbf{X}_{\leq T}) \leq \mathbb{E} [\lambda_{1:k}(\mathbf{X}_{\leq T} + \mathbf{N}_T)]$ and hence:

$$\begin{aligned}\lambda_{1:k}(\mathbf{X}_{\leq T}) &\leq \sum_{t=1}^T \mathbb{E} [\text{tr}(\tilde{\mathbf{P}}_t(\mathbf{X}_t + \mathbf{N}_t - \mathbf{N}_{t-1}))] \\ &\leq \sum_{t=1}^T \mathbb{E} [\text{tr}(\tilde{\mathbf{P}}_t \mathbf{X}_t)] + \sum_{t=1}^T \mathbb{E} \left[\max_{\mathbf{P} \in \mathcal{P}} \{\mathbf{N}_t - \mathbf{N}_{t-1}\} \right] \\ &= \sum_{t=1}^T \mathbb{E} [\text{tr}(\tilde{\mathbf{P}}_t \mathbf{X}_t)] + \sum_{t=1}^T \mathbb{E} [\lambda_{1:k}(\mathbf{N}_t - \mathbf{N}_{t-1})].\end{aligned}$$

The lemma follows by plugging the inequality above into the definition of the regret (1).

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